

The Green Lab Notebook:

***Chemical intelligence and green informatics
in a mobile app***

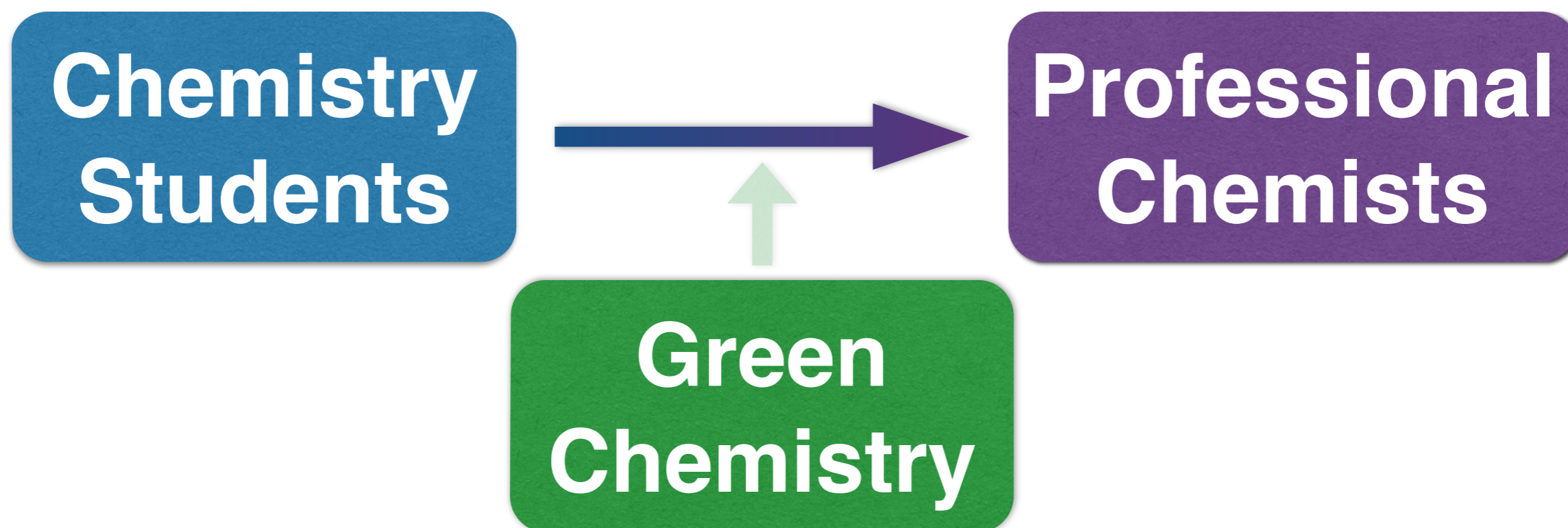
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Alex M. Clark**

July 2014



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<http://molmatinf.com>



- **Green chemistry** is like a distinct profession:
 - its own journals, grants, conferences...
- **Students** need to develop habits early
- **Professionals** need information access

Software Can Help

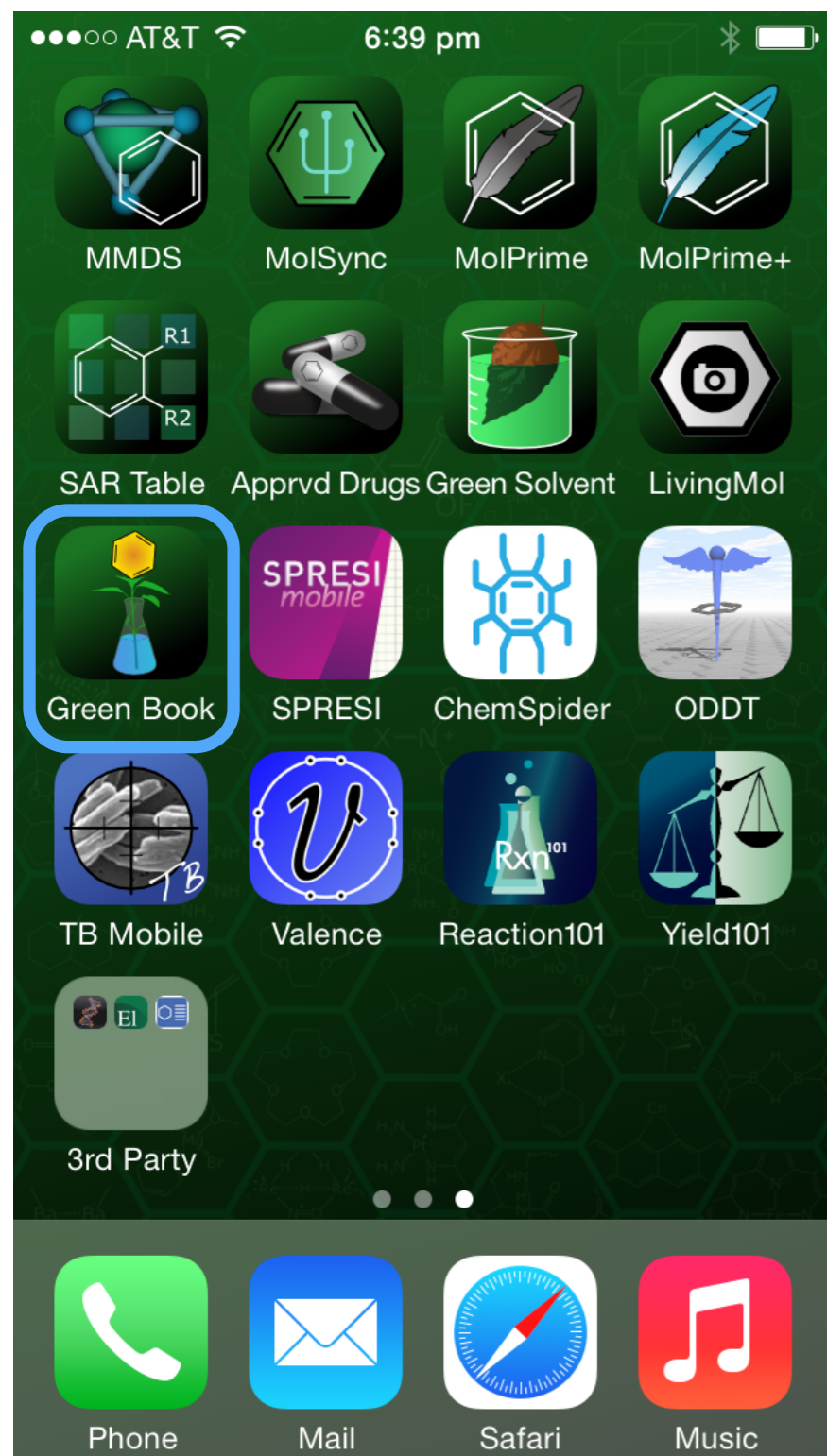
Calculations

- percentage yield
- atom efficiency
- process mass intensity
- E-factor

Information

- greener solvents
- sustainable feedstocks
- hazardous byproducts
- benign reactions

Mobile App



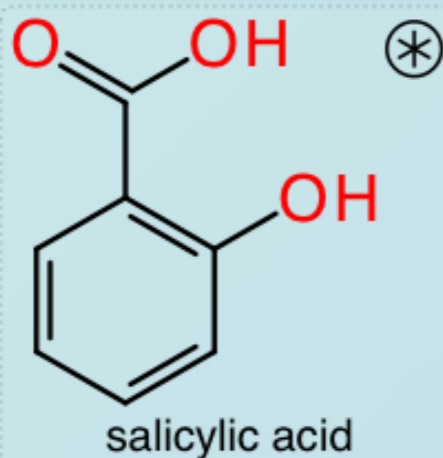
- Mobile: the platform of the future
- Where the action is: UX/UI innovation
- Where the students are now: iPhones, iPads, etc.
- Needs to be accessible, affordable, simple, effective...

Making Aspirin

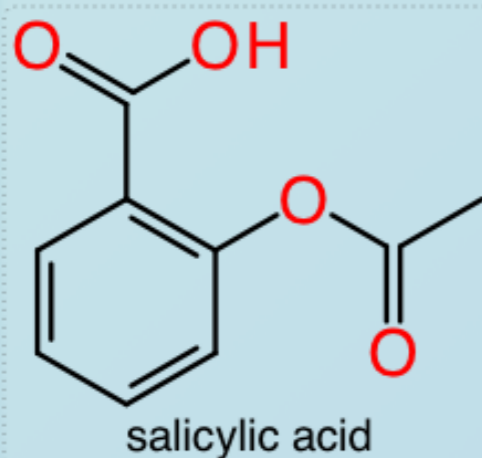
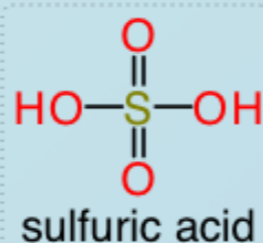
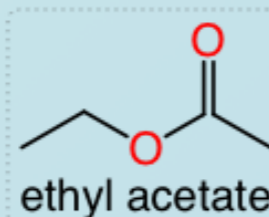
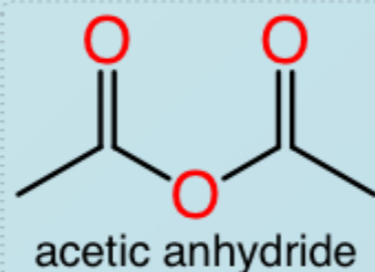
Edit Experiment

Acetylation to make aspirin

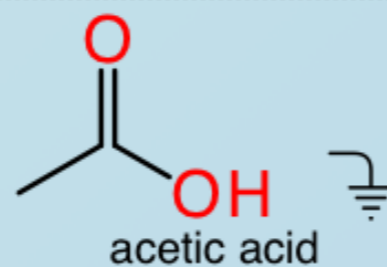
28/05/2014
22/06/2014



+



+



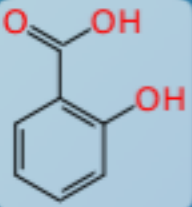
- The quintessential undergraduate reaction...

Reactants

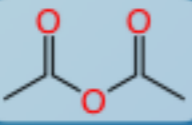
Reagents

Products

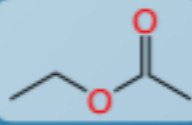
Entering Quantities



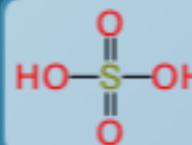
Equiv:	1
MW:	138.121 g/mol
Mass:	2 g
Volume:	
Moles:	0.0144801 mol
Density:	
Conc:	



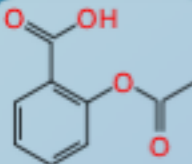
Equiv:	1
MW:	102.089 g/mol
Mass:	5.4 g
Volume:	5 mL
Moles:	0.0528952 mol
Density:	1.08 g/mL
Conc:	



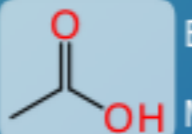
Equiv:	88.378
MW:	88.1051 g/mol
Mass:	112.75 g
Volume:	125 mL
Moles:	1.27972 mol
Density:	0.902 g/mL
Conc:	



Equiv:	0.00704134
MW:	98.0785 g/mol
Mass:	0.01 g
Volume:	
Moles:	0.101959 mmol
Density:	
Conc:	



Equiv:	1
MW:	180.157 g/mol
Mass:	2.1 g
Volume:	
Moles:	0.0116565 mol
Density:	
Conc:	
Yield:	80.5 %



Equiv:	1
MW:	60.052 g/mol
Mass:	0.869557 g
Volume:	
Moles:	0.0144801 mol
Density:	
Conc:	
Yield:	

- Use the app to enter quantities for each reaction component

- Automagic calculation of **molecular weight**, **moles**, **volume** ↔ **mass** (*density, concentration*), **yield**

Calculations

Yield

actual product amount

theoretical product amount

 **100%**

Atom Economy

Σ **product molecular weight**

Σ **reactant molecular weight**

 **100%**

Process Mass Intensity

Σ **reactant mass**

Σ **product mass**

 **1**

E-factor

Σ **waste mass**

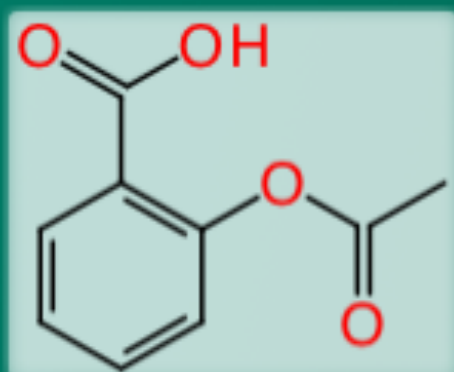
Σ **product mass**

 **0**

Automatic Green Metrics

- Green metrics are *always calculated...*

Σ reactants = 2 g + 5.4 g + 112.75 g + 0.01 g = 120.16 g Σ products = 2.1 g = 2.1 g Σ waste = 0.869557 g = 0.869557 g



$$\text{PMI} = \frac{2 \text{ g} + 5.4 \text{ g} + 112.75 \text{ g} + 0.01 \text{ g}}{2.1 \text{ g}} = 57.2191$$

$$\text{E-factor} = \frac{0.869557 \text{ g} + 117.19 \text{ g}}{2.1 \text{ g}} = 56.2191$$

$$\text{Atom-E} = \frac{180.157}{138.121 + 102.089} = 75.0002 \%$$

- ... always shown, always stored
- These metrics become as accessible as yield
- Easier to compare & optimise for greenness

Solvents

- Choice of solvent has a huge impact on green profile
- Curated data regarding:



Safety



Health



Flammability



Environmental impact



Waste disposal



Reactivity



Lifecycle

Carrier 6 3.8:36 pm Density: 0.791 g/mL

Solvents

t-Butanol

CC(C)(C)O

Class: Alcohol
CASRN: 75-65-0
CSID: 6146
MP: 25 °C
BP: 82 °C
Density: 0.775 g/mL

3 5
 5 3.5
 7 1
 3

Benzene

c1ccccc1

Class: Aromatic
CASRN: 71-43-2
CSID: 236
MP: 6 °C
BP: 80 °C
Density: 0.874 g/mL

5 10
 8 5.5
 4 1
 4

Toluene

Cc1ccccc1

Class: Aromatic
CASRN: 108-88-3
CSID: 1108
MP: -95 °C
BP: 111 °C
Density: 0.865 g/mL

5 7
 7 6.5
 3.5 1
 4

Using Solvents

Edit Experiment

Acetylation to make aspirin 22/06/2014

Select known solvent.

ethyl acetate

sulfuric acid

salicylic acid

acetic acid

Select from Solvents

Butyl acetate

Dimethyl carbonate

Ethyl acetate

Ethyl formate

Ethyl lactate

Ethyl acetate

Equiv:	88.378
MW:	88.1051 g/mol
Mass:	112.75 g
Volume:	125 mL
Moles:	1.27972 mol
Density:	0.902 g/mL
Conc:	

Sulfuric acid

Equiv:	0.00704134
MW:	98.0785 g/mol
Mass:	0.01 g
Volume:	
Moles:	0.101959 mmol
Density:	
Conc:	

Feedstocks

Common Feedstocks

- ethanol**
Source: Fermentation
CCO
- glucose**
Source: Biomass
C1C(C(C(C(C(O1)O)O)O)O)O
- butanol**
Source: Fermentation
CCCCO
- thiophene**
Source: Fossil
C1=CC=C(S1)
- glycine**
Source: Biomass
NC(=O)O

- Not all starting materials are created equal
- Some can be made from renewable sources
- Lab notebook is a chance to guide & educate
- Curation is a work in progress...

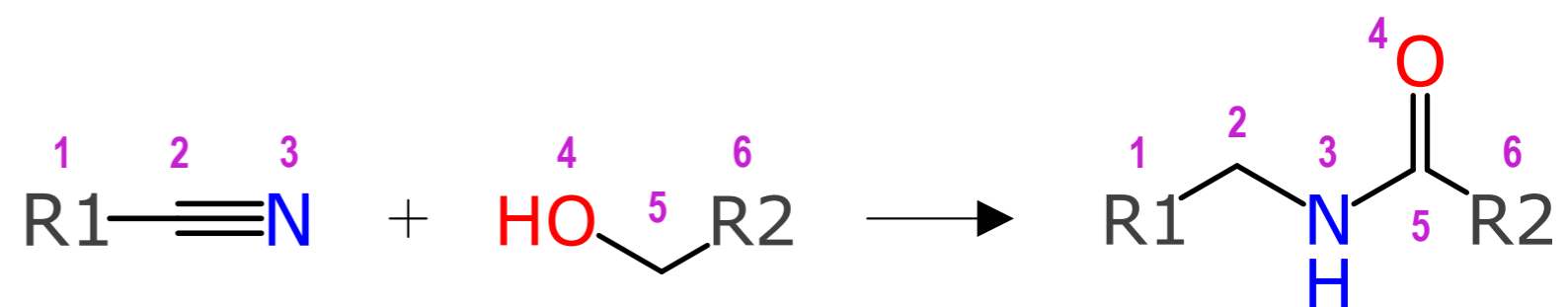
Transforms

Carrier 3:14 PM

Transforms

A_B Strem 1

A_B Strem 2



- Chemical reactions can be curated as *transforms*
- Can be used to search for ways to design a reaction
- Curation of **green transforms** is a way to encourage preferred reaction pathways

Availability

- The **Green Lab Notebook** (GLN) app should be in the iTunes AppStore by autumn
- For iPhones, iPods & iPads
- In the meanwhile, check out:



Green Solvents



Reaction101



Lab Solvents



Yield101

Acknowledgments

- Sean Ekins (Green Solvents)
- Inquiries to **info@molmatinf.com**

**MOLECULAR
MATERIALS
INFORMATICS**

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